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Date: Wed, 23 Feb 2005 07:44:53 -0500
To: hhasan@nasa.gov, Theresa.A.Bryant@nasa.gov
From: Barbara Dreyfus <bmd@pha.jhu.edu>
Subject: Annual technical report for NAG5-13114
Cc: sormond@jhu.edu, skain@pha.jhu.edu, neufeld@pha.jhu.edu, bmd@pha.jhu.edu

I am forwarding the following on behalf of Professor David Neufeld. Please let me know if you require anything further. Thank you. Barbara Dreyfus

From: "David Neufeld" <neufeld@pha.jhu.edu>
To: "Barbara Dreyfus" <bmd@pha.jhu.edu>
Subject: LTSA interim report, NAG5-13114
Date: Tue, 22 Feb 2005 17:03:59 -0500
X-Mailer: Microsoft Outlook Express 6.00.2600.0000

Subject: Annual progress report for Year 2 of my LTSA program, NAG5-13114

Dear Ms. Bryant:

Please find attached in pdf format the annual progress report for Year 2 of my LTSA program.

Please let me know if you require any further materials (e.g. reprints/preprints or more detailed descriptions of the research) at this time.

Sincerely,

David Neufeld

cc: S. Ormond, BARA
S. Kain, P&A
File: D32-2184

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Neufeld Year 2 LTSA annual report1.pdf

Annual progress report for the LTSA program "Molecular Astrophysics from Space: the physical and chemical effects of star formation and the destruction of planetary systems around evolved stars": Year 2

(P.I., David Neufeld, Johns Hopkins University)

During Year 2 of my LTSA program, I have continued to press forward in several of the research directions described in my LTSA proposal.

This year has been noteworthy for the availability of our first Spitzer data, and for the appointment of Dr. Paule Sonnentrucker as an associate research scientist supported by this grant. With extensive experience in ultraviolet absorption line spectroscopy of molecules with FUSE – and in the study of the diffuse interstellar bands – Paule brings a valuable broadening of the expertise available to pursue this LTSA program. Her appointment started 2004 Sep 15.

1. Warm molecular gas in the interstellar medium (ISM)

Our study of IC443 (described in last year's annual report) has been completed, and a paper describing the work has now been accepted for publication in ApJ. We successfully proposed a Spitzer Cycle 1 GO program (P.I., Neufeld) to follow up our SWAS and ISO results with IRS (Infrared Spectrograph) observations of IC443 and 3 other molecular supernova remnants. The Spitzer observations will be started on 2005 Mar 14.

Data are now available from our Spitzer GT program to study line emission from molecular hydrogen and water vapor in warm (400 – 1000 K) interstellar gas. As described in the LTSA proposal, this specific program involves spectral line mapping several interstellar sources chosen to reflect the diversity of interstellar environments. The sources now available are: HH54 and HH7-11, two Herbig-Haro objects, the former being the first object in which a non-equilibrium H₂ ortho-to-para ratio was observed; NGC 7023, a reflection nebula; and Cepheus A, a classic outflow region in which SWAS observations have suggested an enhanced abundance of water vapor

Over the past year, we (Neufeld and Sonnentrucker) have been working intensively with members of the IRS instrument team at Rochester to develop ancillary software needed to construct spectral line maps. We have recently obtained our first such maps, which show the distribution of emission in eight pure rotational lines of molecular hydrogen toward the source HH54. Surprisingly, the results imply that a remarkably constant mixture of gas temperatures is present at all positions within the source, while the ortho-to-para ratio shows significant and varying departures from equilibrium. Further analysis of this dataset is ongoing.

Preliminary results on other sources indicate the presence of strong emission in several mid-IR bands from polycyclic aromatic hydrocarbons (PAHs) in NGC 7023; and

suggest the presence of emission from gaseous carbon dioxide in Cepheus A. These emissions will be mapped along with the molecular hydrogen rotational lines.

We have successfully proposed follow-up observations of four additional sources where warm molecular gas is present: NGC 7538, NGC 2071, BHR 71, and OMC-2. These are currently being carried out as a Spitzer Cycle 1 GO program (P.I., Melnick). We have also very recently proposed a larger (~ 195 hr) Cycle 2 program (P.I., Bergin) to carry out large-scale mapping of warm molecular gas in the Orion and NGC1333 regions where star clusters are forming.

2. Absorption line studies of "cold" molecular clouds

Our Spitzer GT program also included 3 hours devoted to the study of CO₂ ice in gas clouds along sight-lines to field stars. The CO₂ ice observations were carried out in collaboration with Bergin, Melnick, Whittet and Gerakines. CO₂ ice absorption has been detected in the mid-IR spectra of two field stars (Elias 16 and Elias 3), and one protostar (HL Tau); and an upper limit has been obtained toward Tamura 17. These observations indicate that the majority of the CO₂ ice toward Elias 16 is embedded in a polar H₂O-rich ice component, with ~ 15% in an apolar (H₂O-poor) component. This is the first detection of CO₂ in an apolar mantle along the sight-line to a field star. A minimum extinction of $A_V \sim 4$ mag is apparently needed for the onset of CO₂ ice formation, very similar to the threshold found for water ice. These results suggest that CO₂ ice is formed in tandem with water ice. A paper describing the results is almost ready for submission to ApJL. In addition, we successfully proposed a Spitzer Cycle 1 GO program (P.I. Whittet) to follow up this work with observations CO₂ ice towards a larger sample of (~ 50) stars.

In addition to probing the ice component in cold molecular clouds, we have continued to study the gas-phase as well. Sonnentrucker has undertaken an observational study of the physical conditions (local temperature, density, radiation field) prevalent in the diffuse molecular interstellar medium (ISM), using molecular tracers such as H₂, CO, C₂, C₃, CH, CH⁺ and CN. The work was carried out by combining FUV data from the FUSE, HST, and IUE space observatories with high- and medium-resolution ground-based optical data obtained with the McDonald, Kitt Peak and Apache Point Observatory telescopes. The results suggest that CO and CN trace molecular gas that is generally denser and colder than that traced by C₂, C₃, CH and H₂ in the 43 sightlines studied. Comparison of the current theoretical predictions with these observations, however, underline the need for developing models capable of incorporating ranges or mixtures of physical conditions in order to predict accurately the atomic and molecular abundances measured in the diffuse ISM.

With Wolfire and Schilke, Neufeld has completed theoretical investigation of the chemistry of fluorine-bearing molecules in diffuse and dense interstellar gas clouds, combining recent estimates for the rates of relevant chemical reactions with a self-consistent model for the physical and chemical conditions within gas clouds that are exposed to the interstellar ultraviolet radiation field. The study was motivated by the discovery of interstellar HF by ISO and the prospects for future observations with SOFIA and Herschel. We found the chemistry of

interstellar fluorine to be qualitatively different from that of any other element, because – unlike the atoms of any other element found in diffuse or dense molecular clouds – atomic fluorine undergoes an exothermic reaction with molecular hydrogen. Over a wide range of conditions attained within interstellar gas clouds, the product of that reaction – hydrogen fluoride – is predicted to be the dominant gas-phase reservoir of interstellar fluorine nuclei. Fluorine is the heavy element that shows the greatest tendency toward molecule formation; in diffuse clouds of small extinction, the predicted HF abundance can even exceed that of CO, even though the gas-phase fluorine abundance is four orders of magnitude smaller than that of carbon. Our model predicts HF column densities $\sim 10^{13} \text{ cm}^{-2}$ in dark clouds and column densities as large as 10^{11} cm^{-2} in diffuse interstellar gas clouds with total visual extinctions as small as 0.1 mag. Such diffuse clouds will be detectable by means of absorption line spectroscopy of the $J = 1 - 0$ transition at $243.2 \mu\text{m}$ using SOFIA and Herschel. This raises the interesting (and surprising) possibility that spectroscopic observations of far-infrared continuum sources with SOFIA and HSO will reveal a component of foreground molecular gas that is observable exclusively by means of its HF absorption lines. A paper describing this study has recently been submitted to ApJ.

3. Vaporization of comets around the AGB star IRC+10216

Following up on our detection of H_2CO in the carbon-rich AGB star IRC+10216, we (Schilke, Ford, Neufeld and Melnick) have successfully proposed to search for HDCO at the IRAM 30m telescope. The detection of HDCO would be a definitive proof of our hypothesis that the vaporization of comets is the origin of the H_2O detected by SWAS and the H_2CO detected by IRAM. The observations will be carried out by Paule Sonnentrucker in 2005 Apr 5 – 11.

I have also begun work with F. Bensch on further modeling of the H_2O emission from IRC+10216. This effort will make use of an excitation code developed previously by Bensch to model water emissions from comets. The goal is to obtain predictions for the far-IR water line fluxes that will be measured by the Herschel Space Observatory.

Cumulative list of publications supported fully or partially by this program:

"Water Absorption from Line-of-Sight Clouds toward W49A," Plume, R., Kaufman, M. J., Neufeld, D. A., Snell, R. L., Hollenbach, D. J., Goldsmith, P. F., Howe, J., Bergin, E. A., Melnick, G. J., & Bensch, F. 2004, ApJ, 605, 247 – 258.

"Detection of Formaldehyde toward the Extreme Carbon Star IRC +10216," Ford, K. E. S., Neufeld, D. A., Schilke, P., & Melnick, G. J. 2004, ApJ, 614, 990 – 1006.

"Detection of Water in the Shocked Gas Associated with IC 443: Constraints on Shock Models," Snell, R. L., Hollenbach, D., Howe, J. E., Neufeld, D. A., Kaufman, M. J., Melnick, G. J., Bergin, E. A., & Wang, Z. 2005, ApJ, 620, 758 – 773

"The Chemistry of Fluorine-Bearing Molecules in Diffuse and Dense Interstellar Gas Clouds," Neufeld, D. A., Wolfire M. G., & Schilke, P., 2005, ApJ, submitted